Ethyleneimine 99

_	,			
151-56-4	D	TXS	SID8	02059

Model Performance

_			
N	Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (75	Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 16.2 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.49e-01

Confidence level: 5.83e-01

Nearest Neighbors from the Training Set

Image not found

Ethyleneimine Measured: 23.2 Predicted: 16.2 Image not found

Propyleneimine Measured: 17.5 Predicted: 12.3

Image not found

Pyrrolidine
Measured: 14.1
Predicted: 9.91

Image not found

Pyrrole

Measured: 6.71e-01 Predicted: 2.61 Image not found

Methylamine
Measured: 34.8
Predicted: 25.8